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Pressure swing adsorption (PSA) is a cyclic adsorption process for gas separation and purification with the potential for high productivity compared to alternative separation processes. The design of a cost-competitive and highly productive PSA process requires the optimisation of the process conditions with respect to the usually conflicting objectives purity, recovery and energy consumption. In the usual optimisation approach the governing hyperbolic/parabolic partial differential algebraic equations (PDAE) are simulated to cyclic steady state (CSS) for each parameter set generated by the optimisation routine. Since the system of PDAEs is usually large this approach is computationally very expensive. Thus most optimisation approaches either used simplified governing equations or optimised over a reduced set of parameters. Recently, reduced order and surrogate modelling approaches have been used for the optimisation of PSA systems.

Here we present a surrogate based multi-objective optimisation procedure for the design of PSA systems. This work is an extension of the previous single objective optimisation of the authors [1] to multiple objectives such as purity, recovery and energy consumption. The general idea is to build a surrogate model from a limited number of high-fidelity simulations and to perform the optimisation on the surrogate model. The surrogate is built and updated with design points calculated from our in-house PSA simulator which uses an accurate mathematical model for the dynamics of the PSA system. The NSGA-II multi-objective genetic algorithm is linked to the surrogate to perform the optimisation on the surrogate model; this reduces the computational complexity considerably because the surrogate is computationally less expensive to evaluate compared to the full PSA model. The solution obtained by the surrogate based optimisation procedure is validated against the full model and, if necessary, the NSGA-II optimisation procedure is repeated with an updated surrogate model; using the validation simulations with the full model to update the surrogate.

The resulting surrogate based optimisation outperforms a NSGA-II optimisation linked directly to the full PSA simulator in a case study optimising the separation of a binary gas mixture in a 2 bed, 6 step PSA system. The surrogate based optimisation reaches a more favourable Pareto front than the conventional optimisation with less

than 25% of the high-fidelity model simulations; thus enabling the optimisation of full-scale PSA systems over a large set of parameters and using accurate mathematical models.

[1] J. Beck, D. Friedrich, S. Brandani, S. Guillas, and E. S. Fraga, “Surrogate based Optimisation for Design of Pressure Swing Adsorption Systems,” in *Proceedings of the 22nd European Symposium on Computer Aided Process Engineerin*g, 2012, pp. 1217–1221.